LSC Area Percent Report

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

Integration Parameters: rteint.p
Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF139565.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.175	6	14	31	rVB	1820736	2838636	100.00%	18.777%
2	3.387	215	220	239	rBV	29207	76224	2.69%	0.504%
3	5.093	499	510	518	rBV	83004	127305	4.48%	0.842%
4	5.498	573	579	584	rBV	1209079	1625575	57.27%	10.753%
5	6.504	744	750	755	rBV	1310384	1733547	61.07%	11.467%
6	6.875	808	813	818	rBV	336954	400624	14.11%	2.650%
7	7.434	902	908	914	rBV	782251	1032605	36.38%	6.830%
8	8.157	1025	1031	1047	rVB	419317	514323	18.12%	3.402%
9	8.469	1079	1084	1099	rVB	49662	71031	2.50%	0.470%
10	9.228	1208	1213	1219	rBV	1285887	1667834	58.75%	11.032%
11	9.910	1323	1329	1334	rBV	456729	571071	20.12%	3.777%
12	10.004	1341	1345	1351	rVB	35738	57164	2.01%	0.378%
13	10.316	1395	1398	1402	rBV2	29705	36629	1.29%	0.242%
14	10.698	1458	1463	1469	rBV	846940	1096326	38.62%	7.252%
15	11.398	1577	1582	1590	rBV	474097	608995	21.45%	4.028%
16	11.921	1667	1671	1677	rBV2	58015	95492	3.36%	0.632%
17	12.980	1846	1851	1861	rVB	1366919	1734086	61.09%	11.471%
18	13.880	2000	2004	2017	rVB2	19613	47454	1.67%	0.314%
19	14.033	2025	2030	2042	rVB	310914	412129	14.52%	2.726%
20	15.504	2274	2280	2291	rBV	229652	370666	13.06%	2.452%

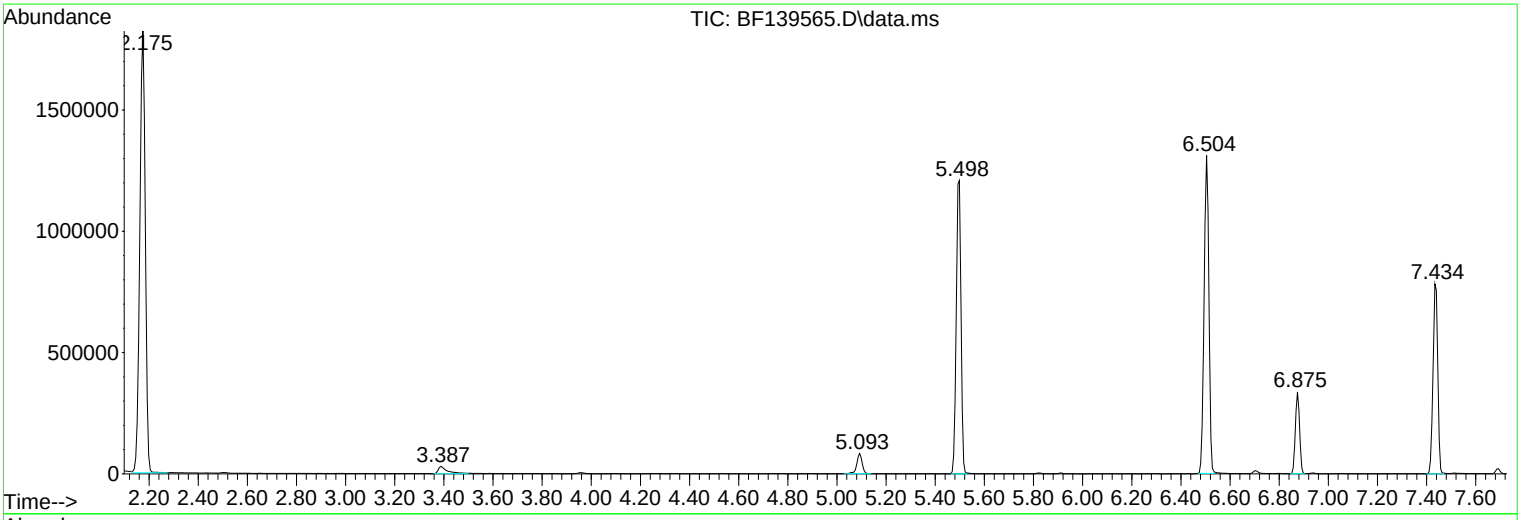
Sum of corrected areas: 15117716

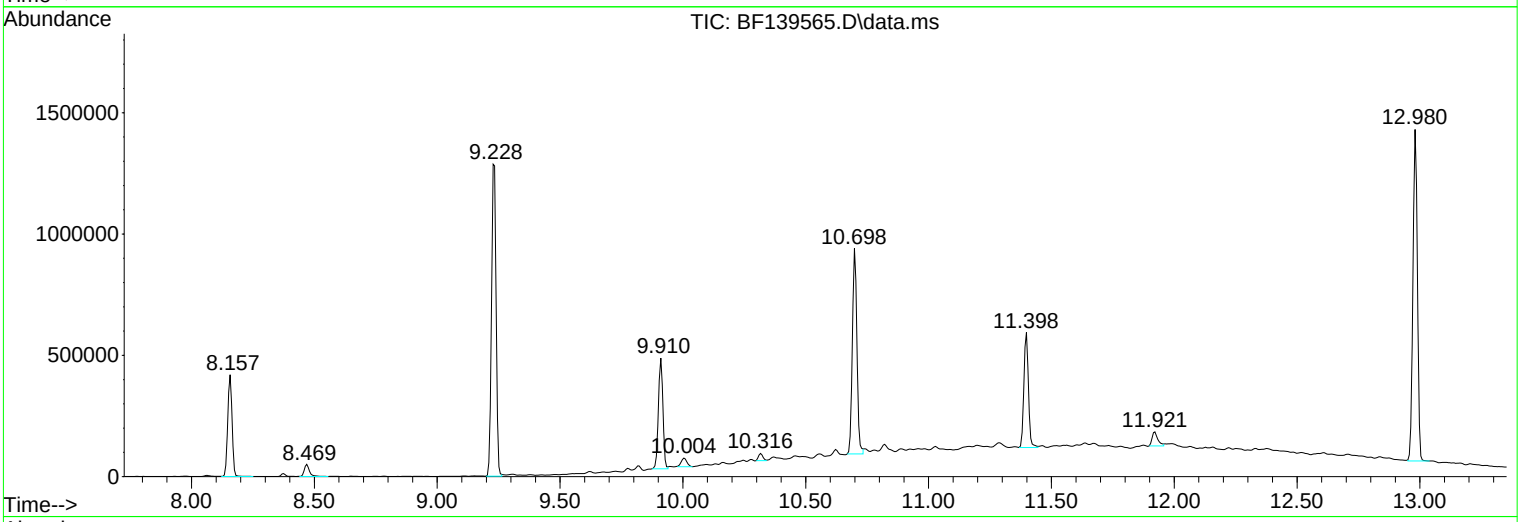
Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

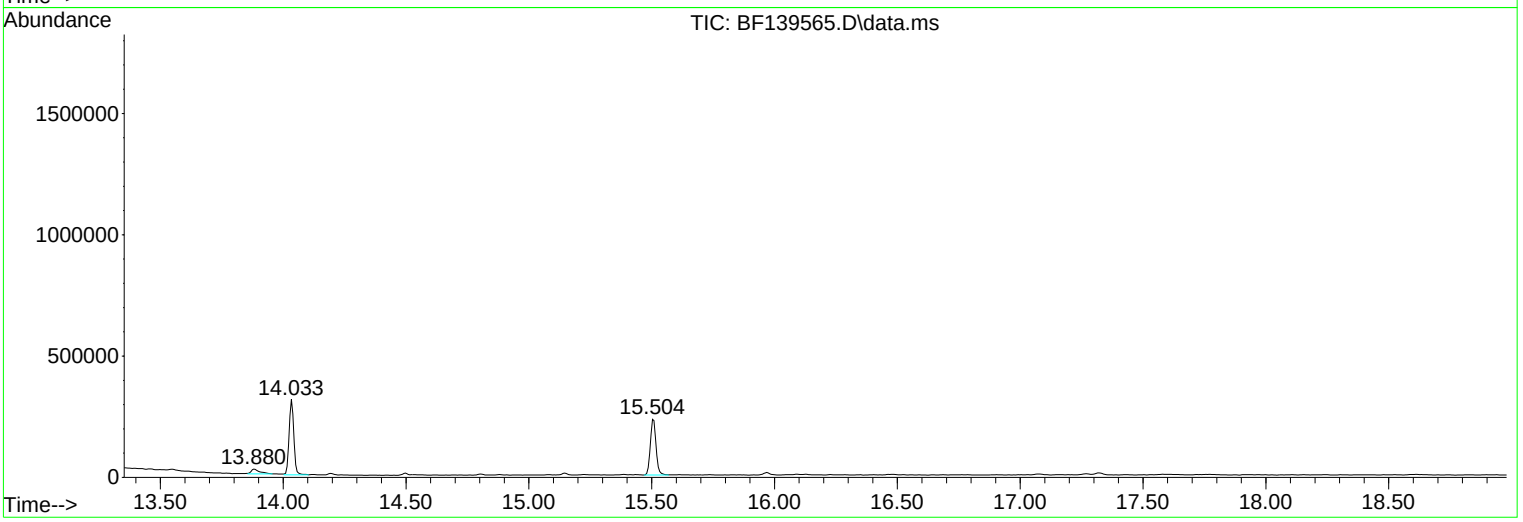
Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P







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Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

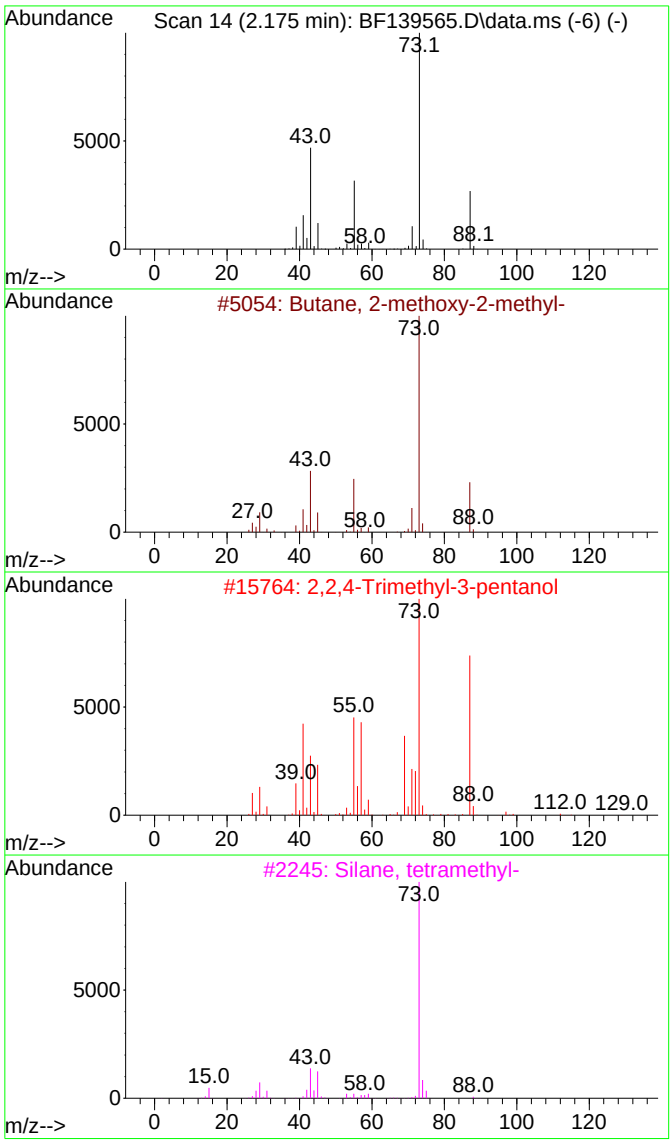
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

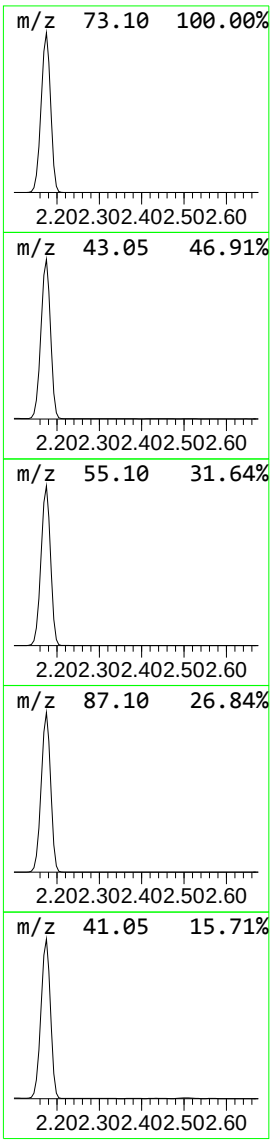
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.175	141.71 ng	2838640	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2	2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3	Silane, tetramethyl-	88	C4H12Si	000075-76-3	38
4	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	23
5	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

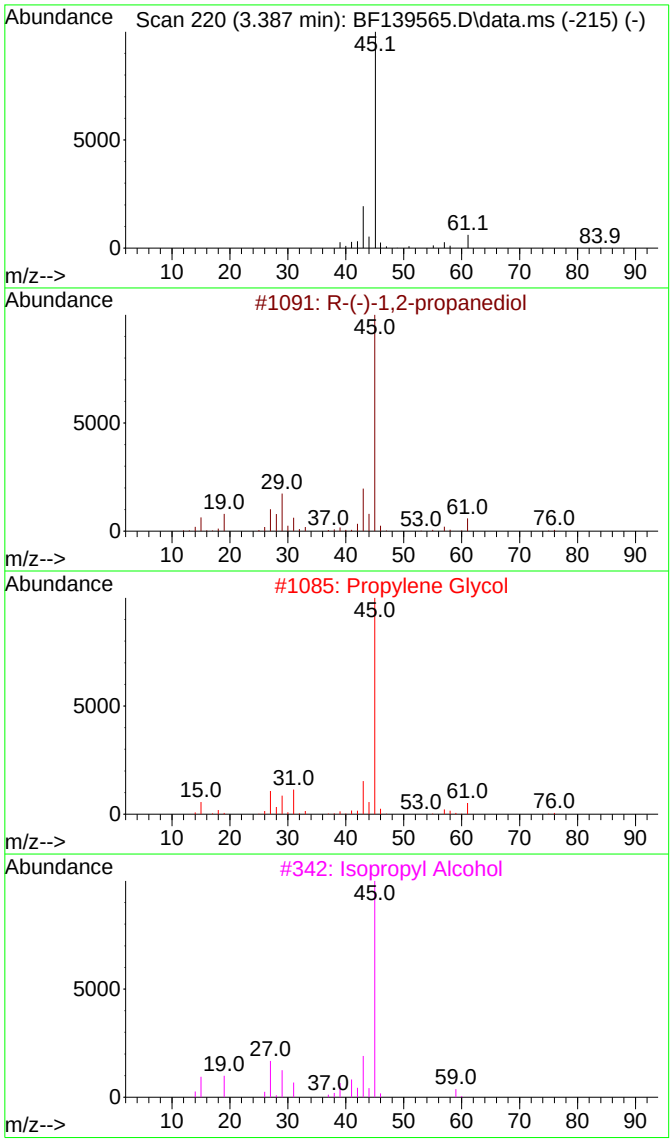
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

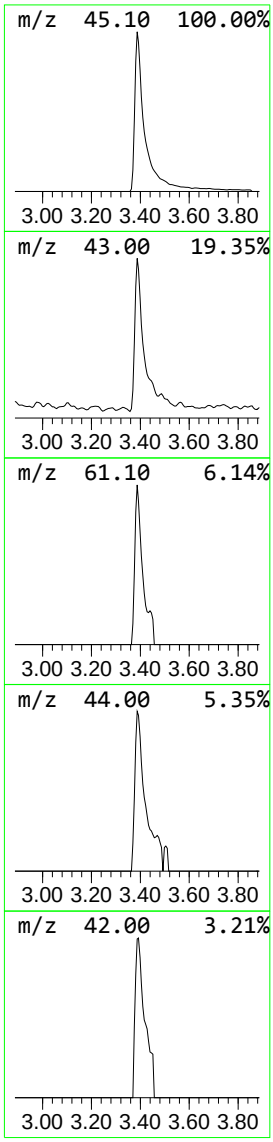
****

Peak Number 2 unknown3.387 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.387	3.81 ng	76224	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
2	Propylene Glycol	76	C3H8O2	000057-55-6	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	Propanoic acid, 2-hydroxy-, meth...	104	C4H8O3	000547-64-8	9
5	(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	9





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

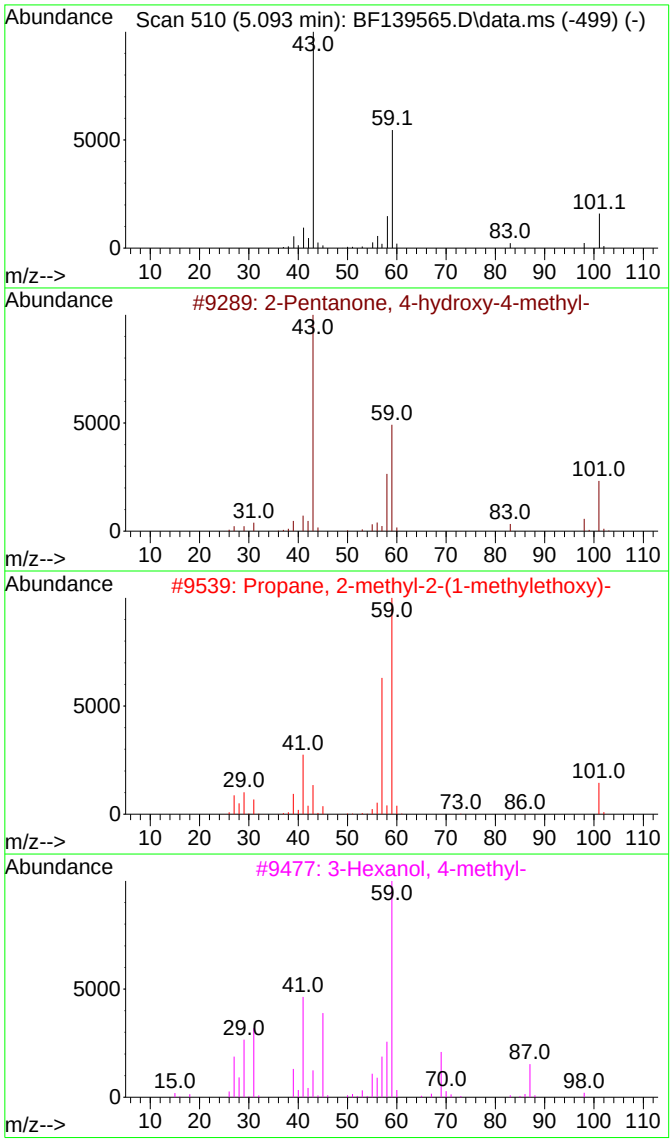
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

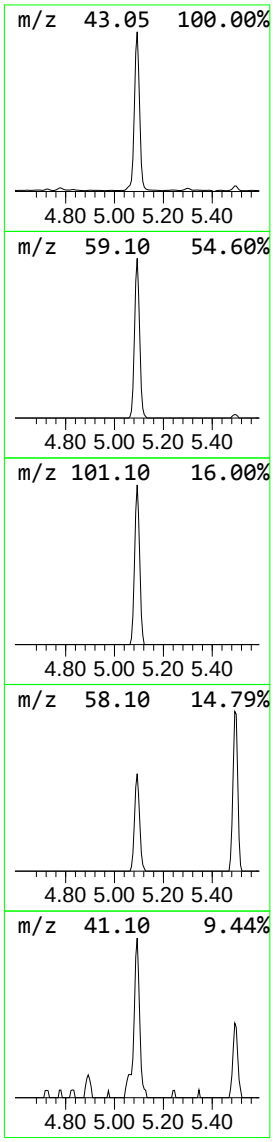
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

****
Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.093	6.36 ng	127305	1,4-Dichlorobenzene-d4	6.875

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5	Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	28





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

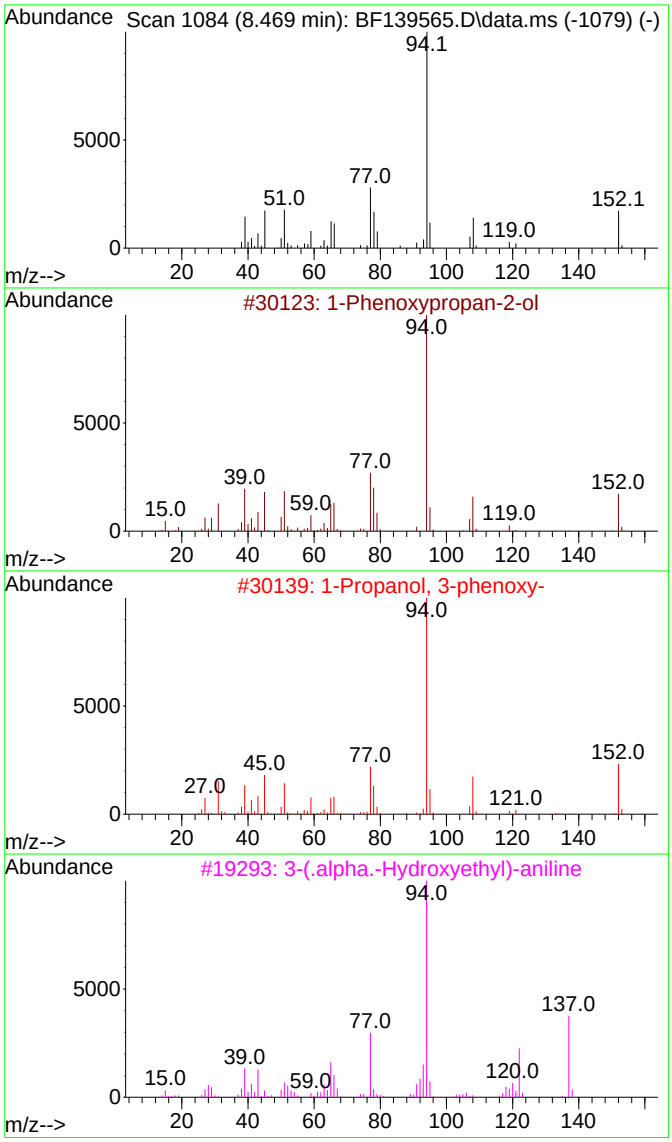
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

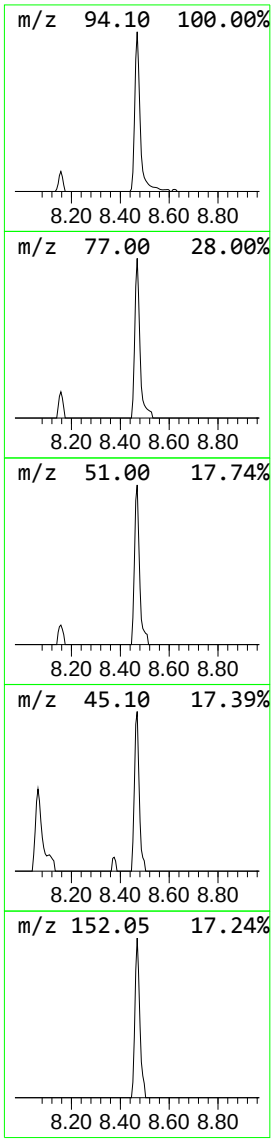
****

Peak Number 4 1-Phenoxypropan-2-ol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.469	2.76 ng	71031	Naphthalene-d8	8.157

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Phenoxypropan-2-ol	152	C9H12O2	000770-35-4	96
2	1-Propanol, 3-phenoxy-	152	C9H12O2	006180-61-6	83
3	3-(.alpha.-Hydroxyethyl)-aniline	137	C8H11NO	002454-37-7	59
4	tert-Butyl phenyl carbonate	194	C11H14O3	006627-89-0	53
5	Benzene, (2-methylpropoxy)-	150	C10H14O	001126-75-6	53





Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

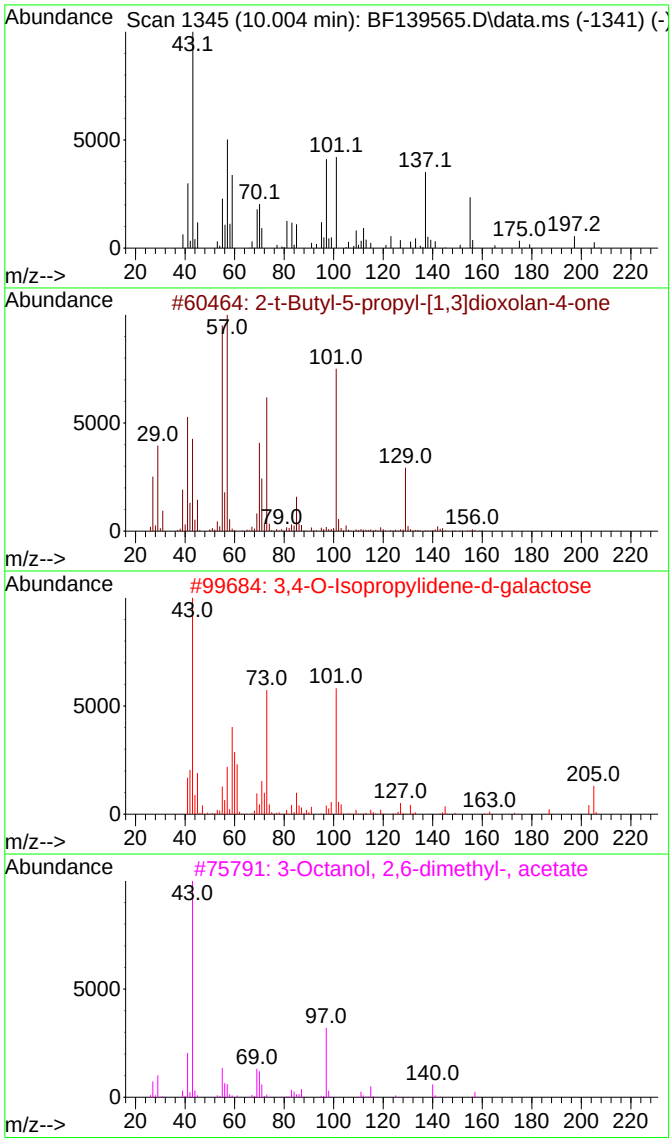
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

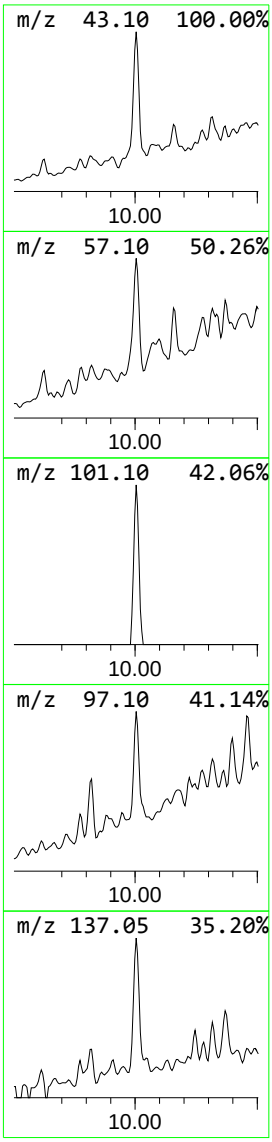
****

Peak Number 5 unknown10.004 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.004	2.00 ng	57164	Acenaphthene-d10	9.910

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-t-Butyl-5-propyl-[1,3]dioxolan...	186	C10H18O3	157733-17-0	12
2	3,4-O-Isopropylidene-d-galactose	220	C9H16O6	1000129-84-6	12
3	3-Octanol, 2,6-dimethyl-, acetate	200	C12H24O2	123232-57-5	10
4	5-Acetyl-2,4-dimethylthiazole	155	C7H9NOS	038205-60-6	10
5	9-Acetoxynonanal	200	C11H20O3	029541-97-7	10





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Data File : BF139565.D
Acq On : 27 Sep 2024 00:16
Operator : RC/JU
Sample : P4198-16
Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

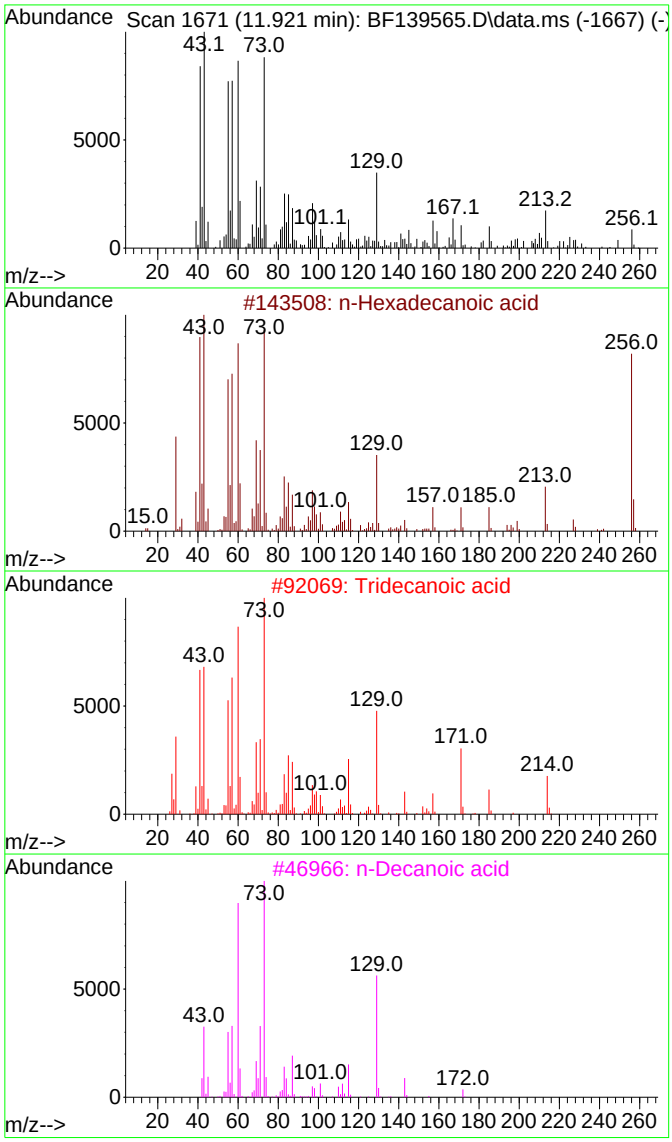
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

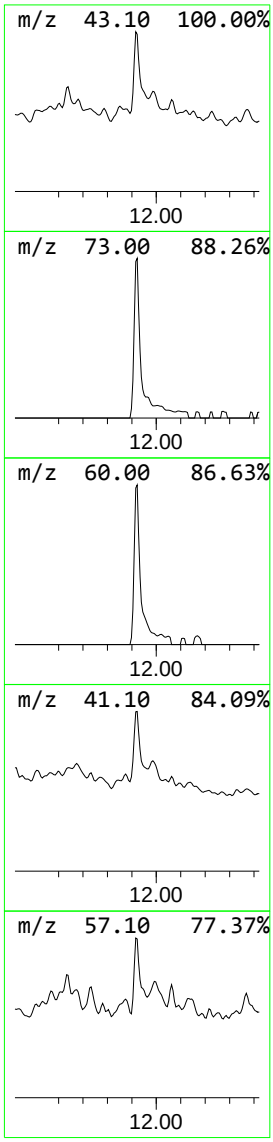
****

Peak Number 6 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.922	3.14 ng	95492	Phenanthrene-d10	11.398

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2	Tridecanoic acid	214	C13H26O2	000638-53-9	92
3	n-Decanoic acid	172	C10H20O2	000334-48-5	91
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	90
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	87





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BNA_F
ClientSampleId :
TP3-WC-1

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF091324.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

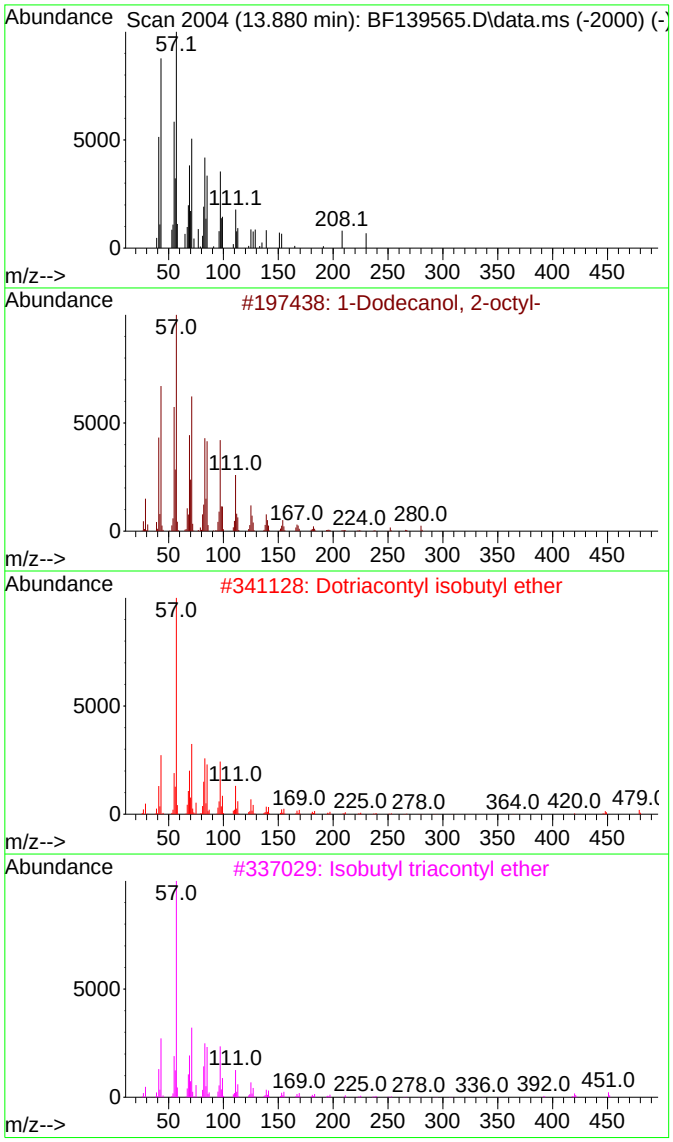
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

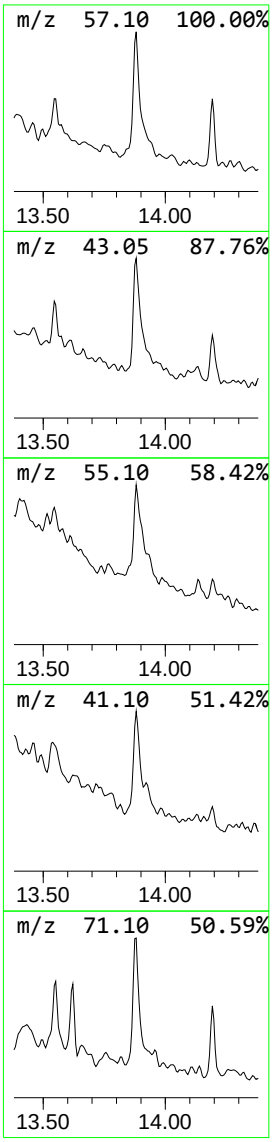
****

Peak Number 7 1-Dodecanol, 2-octyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.880	2.30 ng	47454	Chrysene-d12	14.033

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Dodecanol, 2-octyl-	298	C20H42O	005333-42-6	91
2	Dotriacontyl isobutyl ether	523	C36H74O	1010406-33-6	87
3	Isobutyl triacontyl ether	495	C34H70O	1000406-33-5	87
4	Isobutyl octacosyl ether	467	C32H66O	1000406-33-4	86
5	Hexacosyl isobutyl ether	438	C30H62O	1000406-33-3	86





Tentatively Identified Compound (LSC) summary

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF092624\
Data File : BF139565.D
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Butane, 2-metho...	2.175	141.7	ng	2838640	1	6.875	400624	20.0
unknown3.387	3.387	3.8	ng	76224	1	6.875	400624	20.0
2-Pentanone, 4-...	5.093	6.4	ng	127305	1	6.875	400624	20.0
1-Phenoxypropan...	8.469	2.8	ng	71031	2	8.157	514323	20.0
unknown10.004	10.004	2.0	ng	57164	3	9.910	571071	20.0
n-Hexadecanoic ...	11.922	3.1	ng	95492	4	11.398	608995	20.0
1-Dodecanol, 2-...	13.880	2.3	ng	47454	5	14.033	412129	20.0